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An intersection based ALE scheme (xALE) for cell centered hydrodynamics (CCH)

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Abstract

We extend a cell-centered hydrodynamics method (CCH) [1] on unstructured polyhedral cells to a second-order cell-centered arbitrary Lagrange-Eulerian (ALE) formulation. The method splits the operations into a Lagrange step followed by mesh relaxation and an intersection based remap called xALE. Unlike swept face methods common in Eulerian and ALE schemes [4], intersection methods naturally couple across cell corners. We applied an efficient second-order method of remapping cell centered variables from one unstructured grid to another, based upon seminal work of Dukowicz and Ramshaw (D&R) [2, 3, 8]. The intersection method was later extended to unstructured polygonal grids [5], multiple dimensions [7], and interface reconstruction [6]. Here, we adapt it in a CCH ALE context.

Intersection remap methods have advantages, but are commonly perceived to be computationally expensive. This need not be the case. A new marching front scheme was used to eliminate grid searching. As a result, the computational effort to perform a full intersection remap scales linearly with the number of zones, as opposed to the $N \log N$ scaling typical of intersection based methods. The computational efficiency of the method allows it to also be used in an advection mode in which a relatively small remap is done every cycle. However, unlike swept face methods, there is no inherent time step limitation, and the advection need not be constrained to nearest neighbor cells.

We compare the new remap method with a traditional swept face scheme for several test problems using CCH for the underlying Lagrange step. We identify mesh numerical artifacts in swept face results that are not present in the remap method.

References

- [1] D.E. Burton, T.C. Carney, N. R. Morgan, S.K. Sambastivan, and M.J. Shashkov. A cell-centered Lagrangian Godunov-like method for solid dynamics. *Comput. Fluids*, <http://dx.doi.org/10.1016/j.compfluid.2012.09.008>, 2012.
- [2] J.K. Dukowicz. Conservative rezoning (remapping) for general quadrilateral meshes. *J.Comput.Phys.*,54:411–424,1984.
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- [5] D.S. Miller, D.E. Burton, , and J.S. Oliviera. Efficient second order remapping on arbitrary two dimensional meshes. Technical Report UCID-ID-123530, available from the authors, Lawrence Livermore National Laboratory, March 1996.
- [6] S.J. Mosso and D.E Burton. Two and three-dimensional interface reconstruction in unstructured meshes. Technical Report LA-UR-00-3522, Los Alamos National Laboratory, October 2000. NECDC, Oakland, October 23-27, 2000.
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- [8] J.D.Ramshaw. Simplified second-order rezoing algorithm for generalized two-dimensional meshes. *J.Comput.Phys.*,67:214–222,1986.

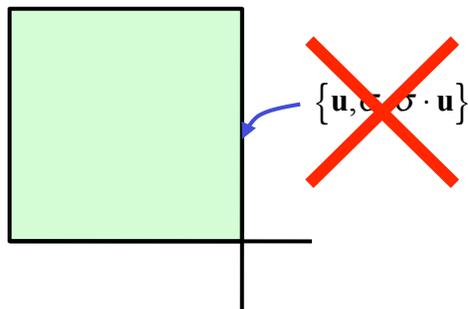
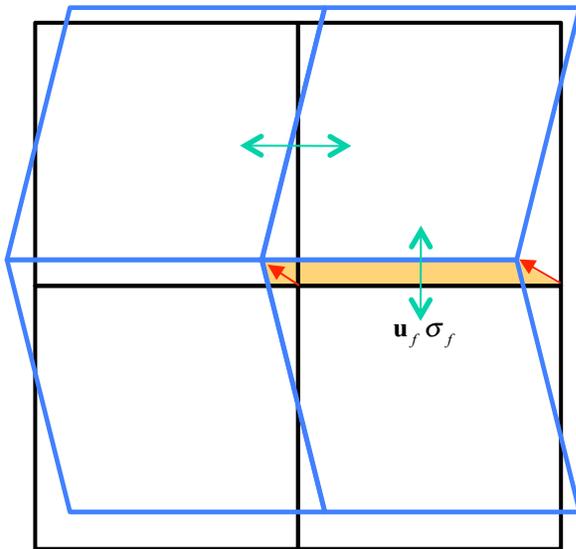
Outline & highlights

- **xALE & eXact intersection remap**
Computational cost $\sim n$
- **Conservation equations**
Alternative equations
- **Monotonicity schemes**
FCT for arbitrary remap
- **Sources of error**
New approach to internal energy
- **Solids**
- **Multi-material formulation**
Multi-material nodal solve
VOF
- **Thoughts to take away**

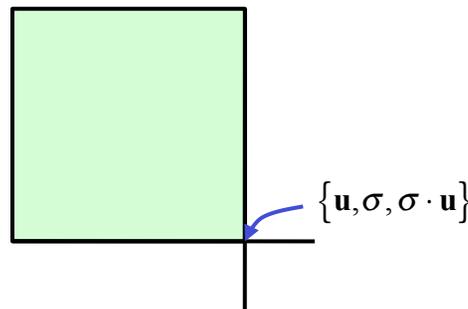
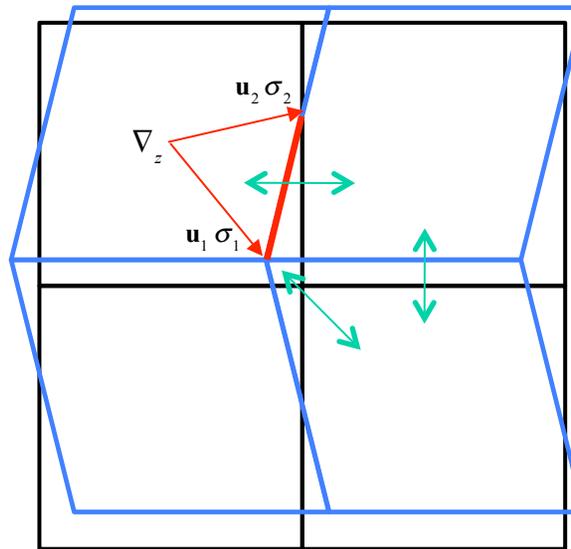
xALE is a cell-centered ALE scheme based on an eXact intersection remap of disparate grids

Swept face advection uses face-centered fluxes

Common in Eulerian & ALE schemes, but does not couple across corners & can violate ancillary relations (e.g. Geometrical Conservation Law - GCL),



Intersection based remap uses second-order integration from intersection to intersection



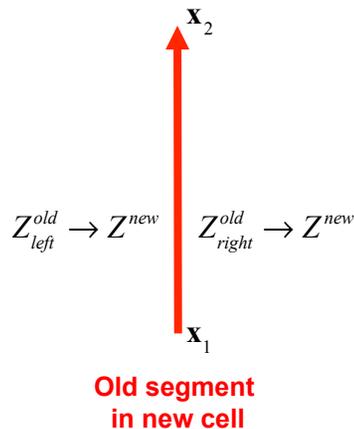
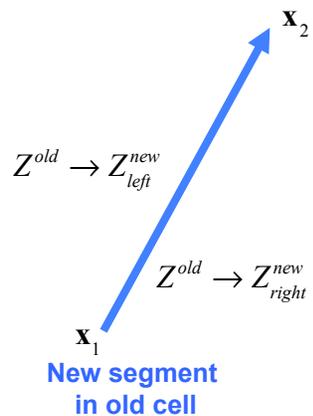
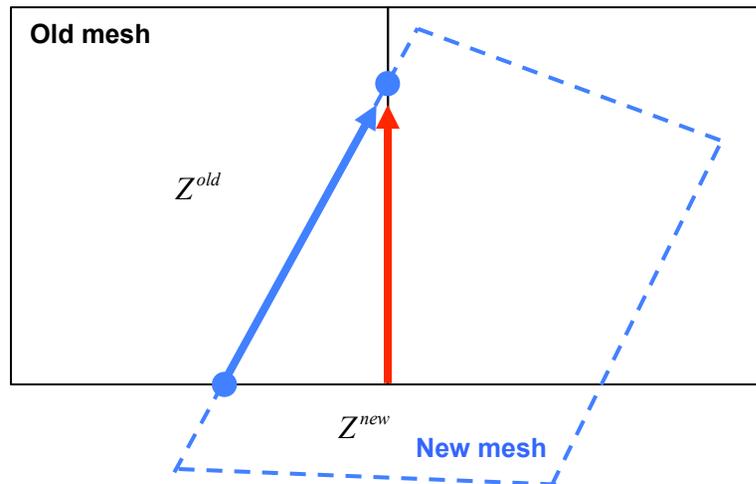
Remap methods are more generally useful

- Not constrained to incremental advection between adjacent cells
- Larger time steps
- Corner coupling
- Second-order integration
- Satisfy ancillary relations

But are perceived to be computationally expensive

- This need not be the case

The second-order remap scheme of Dukowicz & Ramshaw (DR) reduces to a sum of surface fluxes on face segments



A quantity to be remapped ρ is the divergence of some non-unique function \mathbf{f}

$$\rho = \nabla \cdot \mathbf{f}$$

Ramshaw proposed in XY (RZ is similar)

$$\mathbf{f}_x = \frac{1}{2} \mathbf{x} a + \frac{1}{3} \mathbf{x} (\mathbf{x} \cdot \mathbf{b}) + \frac{1}{4} \mathbf{x} (\mathbf{x} \mathbf{x} : \mathbf{c}) + \dots$$

$$a = \rho_z - \mathbf{x}_z \cdot \nabla \rho$$

$$\mathbf{b} = \nabla \rho$$

$$c = 0 \quad (XY)$$

Then the second-order remap quantity can be written as a surface integral

$$\Delta M = \int_{\partial V} \rho \, dv = \oint_{\partial V} d\mathbf{n} \cdot \mathbf{f}$$

$$\rightarrow \sum_i \int_{\partial V} d\mathbf{n} \cdot \mathbf{f} = \sum_i F_i$$

The flux across each segment is given by

$$F_i = \int_i d\mathbf{N} \cdot \mathbf{f} = (\mathbf{N} \cdot \mathbf{x}_1) [aA + \mathbf{b} \cdot \mathbf{B} + c \cdot \mathbf{C} + \dots]$$

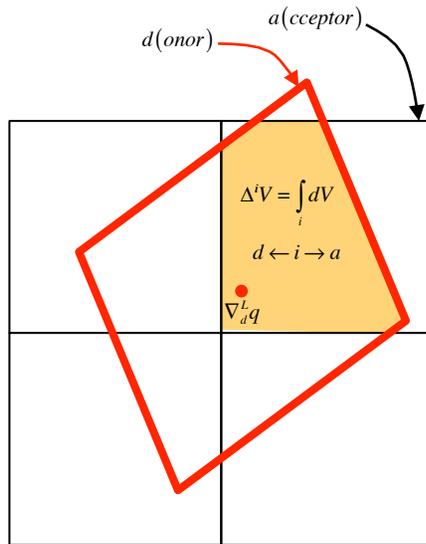
$$A = \frac{1}{2} \int_0^1 ds = \frac{1}{2}$$

$$\mathbf{B} = \frac{1}{3} \int_0^1 ds \mathbf{x} = \frac{1}{3 \cdot 2} (\mathbf{x}_1 + \mathbf{x}_2)$$

$$\mathbf{C} = \frac{1}{4} \int_0^1 ds \mathbf{x} \mathbf{x} = \frac{1}{4 \cdot 3} \left[\mathbf{x}_1 \mathbf{x}_1 + \mathbf{x}_2 \mathbf{x}_2 + \frac{1}{2} (\mathbf{x}_1 \mathbf{x}_2 + \mathbf{x}_2 \mathbf{x}_1) \right]$$

Dukowicz, et al, 1984
 Ramshaw, 1985, 1986
 Miller, Burton, Oliviera 1996
 Mosso, Burton, Harrison 1998
 Mosso, Burton 2000

Discrete form of conservative remap equations for disparate grids – no assumptions of similar connectivity



Conserved quantities

Volume

$$V_a = \sum_i^a \Delta^i V$$

volume flux

Mass

$$\Delta^i M = \rho_d^i \Delta^i V + \mathbf{J}^i \cdot \nabla^L \rho$$

$$\rho_a = \frac{1}{V_a} \sum_i^a \Delta^i M$$

mass flux

Momentum

$$\Delta^i \mathbf{U} = (\rho \mathbf{u})_d^i \Delta^i V + \mathbf{J}^i \cdot \nabla^L (\rho \mathbf{u})$$

$$\mathbf{u}_a = \frac{1}{M_a} \sum_i^a \Delta^i \mathbf{U}$$

Total energy

$$\Delta^i T = (\rho \tau)_d^i \Delta^i V + \mathbf{J}^i \cdot \nabla^L (\rho \tau)$$

$$\tau_a = \frac{1}{M_a} \sum_i^a \Delta^i T$$

Stress

$$\Delta^i \Sigma = (\sigma)_d^i \Delta^i V + \mathbf{J}^i \cdot \nabla^L (\sigma)$$

$$\sigma_a = \frac{1}{V_a} \sum_i^a \Delta^i \Sigma$$

$$\mathbf{d}_a = \text{constant}$$

Supplemental & alternative quantities

Internal and kinetic energy should not be individually conserved

Only total energy should be conserved

Internal energy

$$\Delta^i E = (\rho e)_d^i \Delta^i V + \mathbf{J}^i \cdot \nabla^L (\rho e)$$

$$e_a = \frac{1}{M_a} \sum_i^a \Delta^i E$$

The calculations presented use the canonical **stress advection** equation

Stress is not a conserved quantity and there can be significant error at strong material discontinuities

We are exploring an alternative. Unlike stress, **elastic deformation** is a conserved quantity

Keeping the resulting stress monotonic motivates consideration of **synchronized FCT**

Compliance

$$\gamma^e = \mathbf{d} : \boldsymbol{\sigma}$$

$$\mathbf{d} \rightarrow \mathbf{I} \frac{1}{\mu^2} = \mathbf{I} \frac{1}{(\rho c)^2}$$

$$\Delta^i \mathbf{D} = (\rho \mathbf{d})_d^i \Delta^i V + \mathbf{J}^i \cdot \nabla^L (\rho \mathbf{d})$$

$$\mathbf{d}_a = \frac{1}{M_a} \sum_i^a \Delta^i \mathbf{D}$$

“Elastic” deformation

$$\Delta^i \Gamma = (\rho \gamma^e)_d^i \Delta^i V + \mathbf{J}^i \cdot \nabla^L (\rho \gamma^e)$$

$$\gamma_a^e = \frac{1}{M_a} \sum_i^a \Delta^i \Gamma$$

$$d(\text{onor}) \leftarrow i \rightarrow a(\text{cceptor})$$

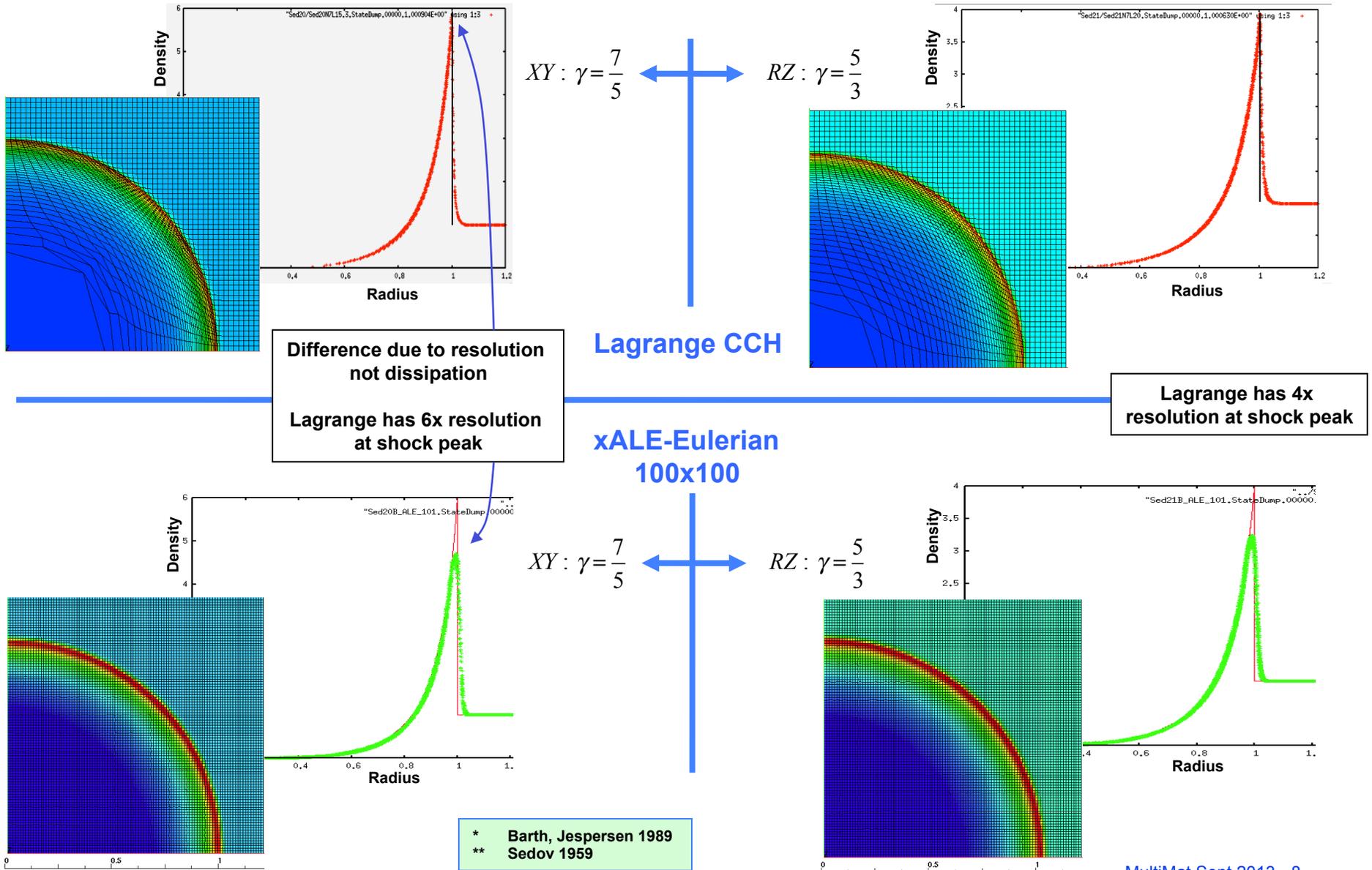
$$(\rho \varphi)_x = (\rho \varphi)_d + (\mathbf{x} - \mathbf{x}_d) \cdot \nabla^L (\rho \varphi)$$

$$\Delta^i V = \int_i dV$$

$$\mathbf{J}^i = \int_i \mathbf{x} dV - \mathbf{x}_d^i \Delta^i V$$

The Dukowicz-Ramshaw equations are used only to calculate these integrals

For a Sedov** blast wave, Lagrange CCH & xALE (BJ*) results compare favorably, but Eulerian requires more resolution to capture the peak

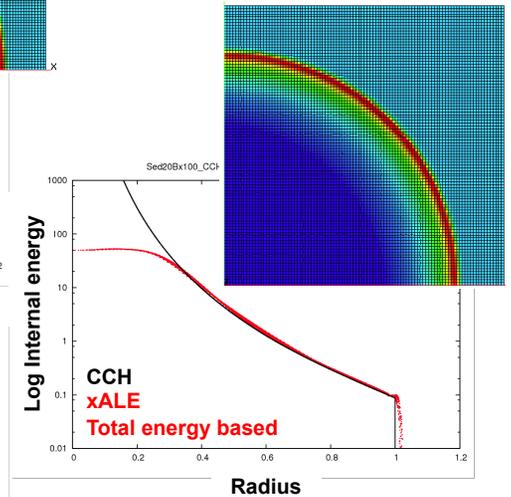
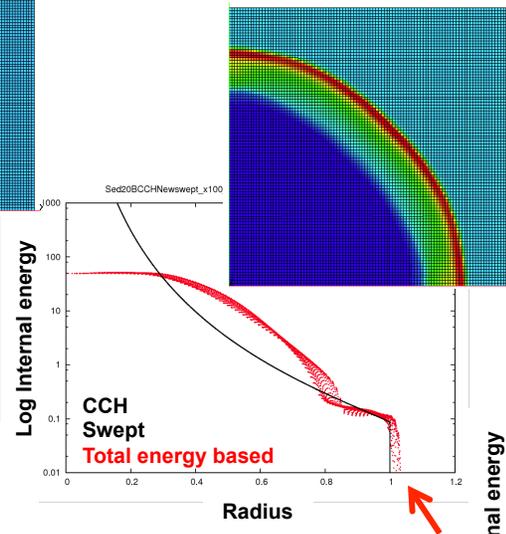
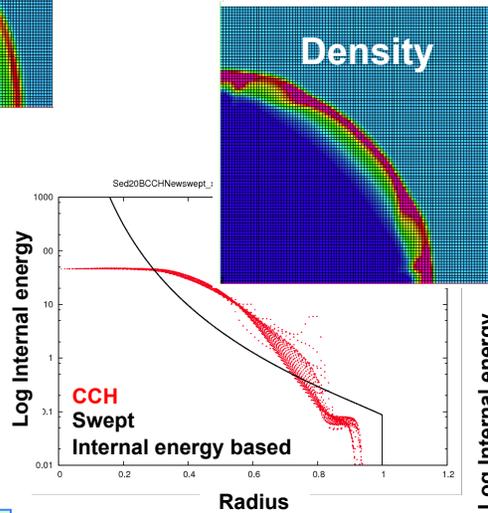
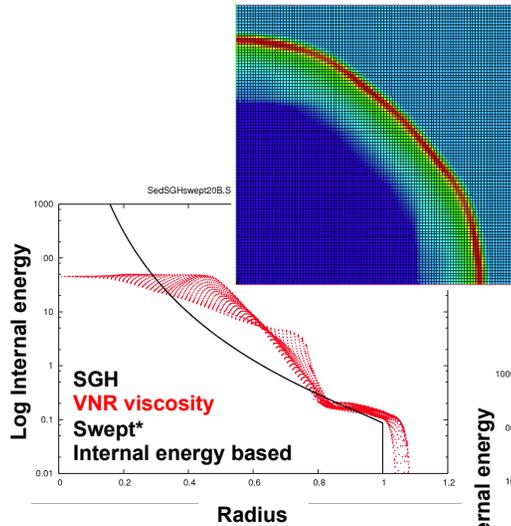


Energy issues

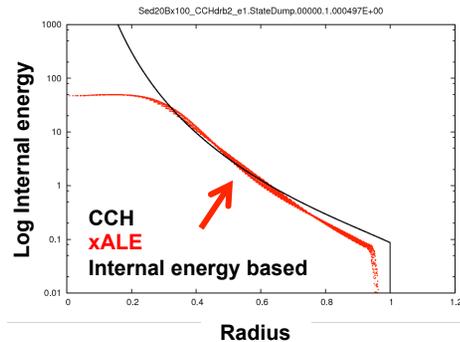
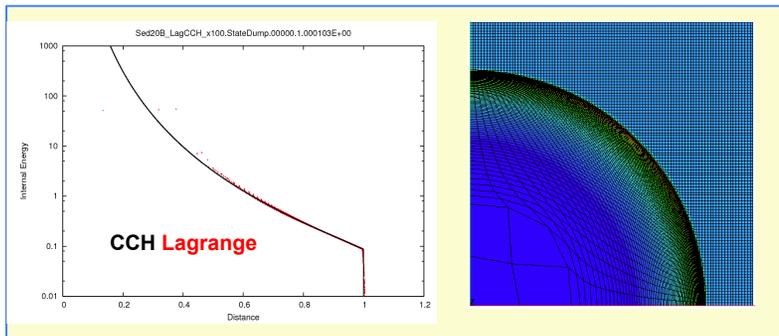
We identified key algorithmic sensitivities in both xALE (BJ) and swept – consider a progression of algorithmic modifications

Question: SGH+swept did not perform well. Why?

Conclusion: both remap and total energy conservation are necessary



* Unsplit advection
Van Leer & FCT limiting
Uniform flux density in swept volumes



Equations for conserved quantities are straightforward, but the proper energy decomposition is less clear: 3 energy formulations

Only total energy should be conserved
Internal and kinetic should not be individually conserved

Advected internal energy

Common in ALE codes

$$k = \frac{1}{2} \mathbf{u}_{adv}^2$$
$$e = e_{adv}$$
$$t = k + e$$

Conserved: e
Not conserved: k, t

e is monotonic - in principle

Problems in shocks
because total energy is not conserved

Example: Sedov

Note: "KE fixup" improves the Sedov problem, but not the Noh problem

Advected total energy

Common in Eulerian codes

$$k = \frac{1}{2} \mathbf{u}_{adv}^2$$
$$t = t_{adv}$$
$$e = t - k$$

Conserved: t
Not conserved: k, e

e is not monotonic

Problems in high velocity & low internal energy regimes
because of the subtraction

Example: Noh

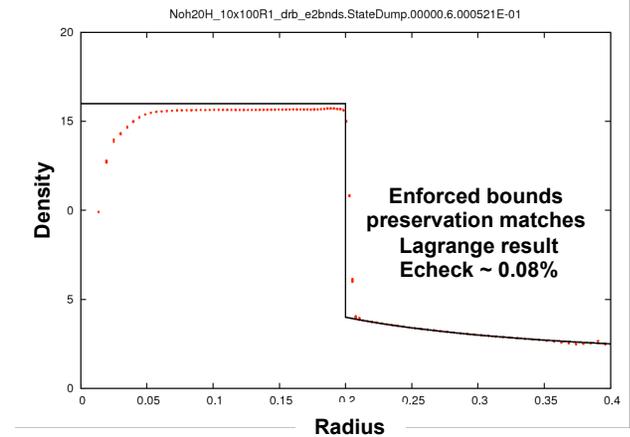
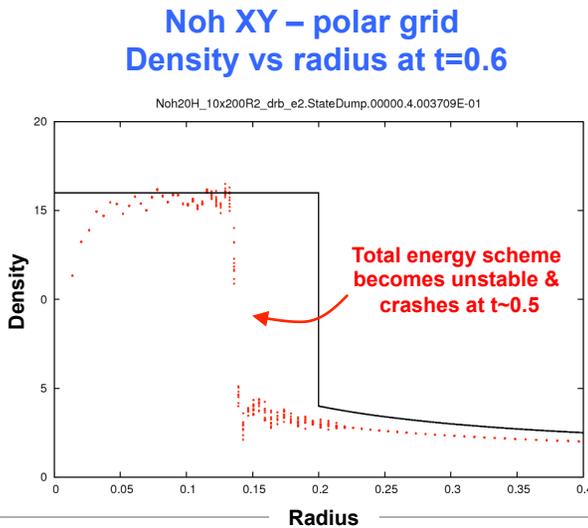
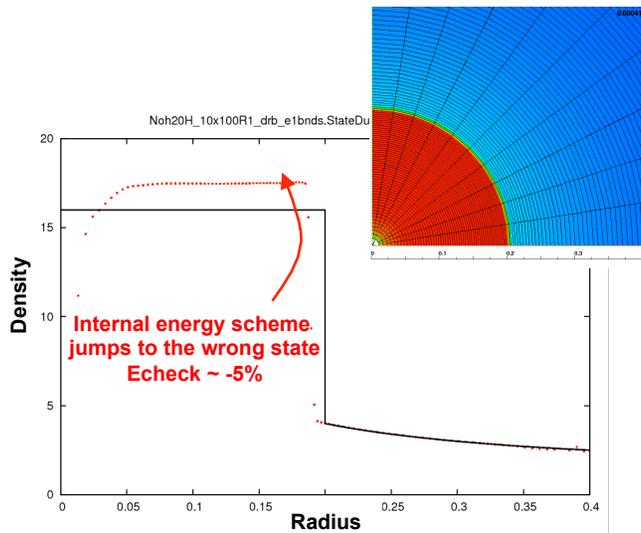
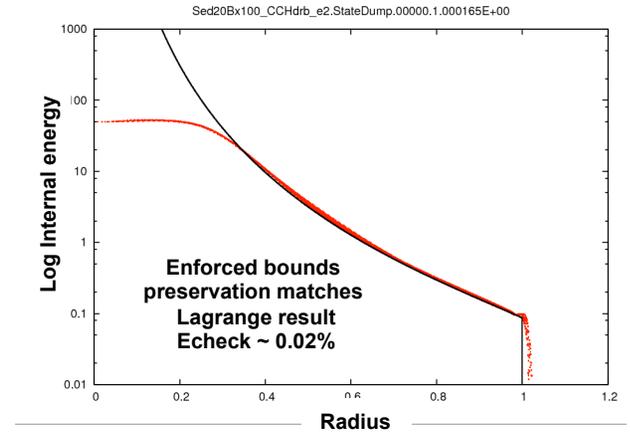
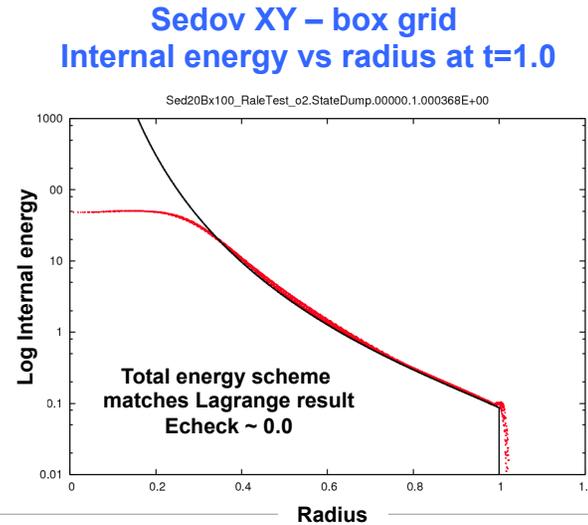
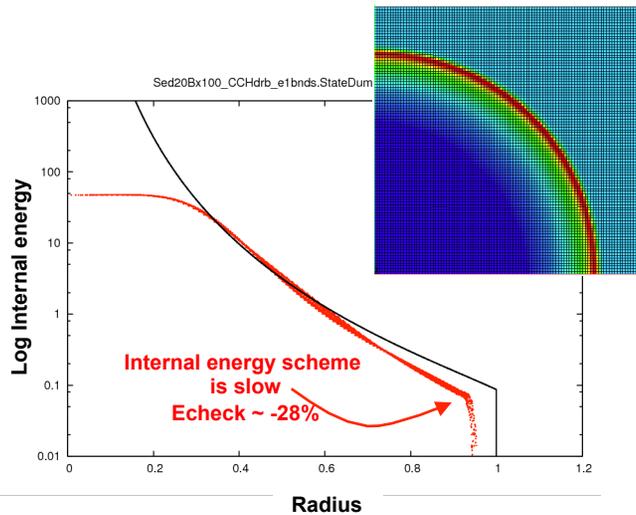
Bounds preservation

By enforcing bounds preservation on the internal energy, the total energy scheme can be made to work in both regimes

This results in a small energy conservation error that is insignificant compared to that associated with the internal energy scheme

An FCT scheme has been proposed by Liska et al that might address the conservation issue

Comparison of 3 energy formulations using CCH and xALE (BJ) – bounds preservation scheme out performs other schemes



Sedov 1959
Noh 1987

Monotonicity

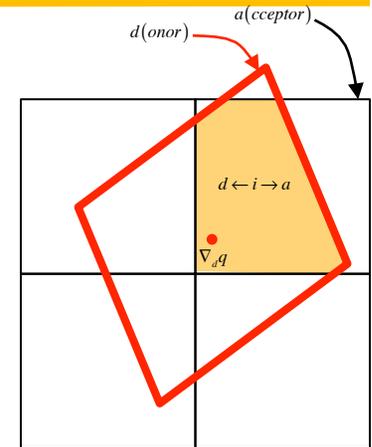
We are working through a progression of monotonicity schemes – FCT can be adapted to ALE remap of disparate grids

- CCH Lagrange hydro, but applicable to SGH
- eXact intersection method as described
- Remap between disparate grids
- Linear reconstruction of conserved variables thru the centroid
- Various internal energy options

$$\rho_x = \rho_d + (\mathbf{x} - \mathbf{x}_d) \cdot \alpha \nabla \rho$$

$$(\rho \mathbf{u})_x = (\rho \mathbf{u})_d + (\mathbf{x} - \mathbf{x}_d) \cdot \beta \nabla (\rho \mathbf{u})$$

$$\mathbf{u}_a = \frac{\int (\rho \mathbf{u})_x dV}{\int \rho_x dV}$$



Unsynchronized: Most of our results are from the first 2 schemes

BJ Barth-Jespersen*

{ $\rho, \rho \mathbf{u}, \dots$ }

Conserved variables are monotonic

{ $\mathbf{u}, \sigma, \dots$ }

Primitive variables are not guaranteed to be monotonic

FCT Basic FCT**

{ α, β }

Limiters for density & other variables are not synchronized

To date, we have not observed this to be a problem, but are concerned about plasticity

S&S Schär-Smolarkiewicz***

{ $\rho, \rho \mathbf{u}, \dots$ }

Conserved variables are monotonic

{ $\mathbf{u}, \sigma, \dots$ }

Primitive variables are monotonic

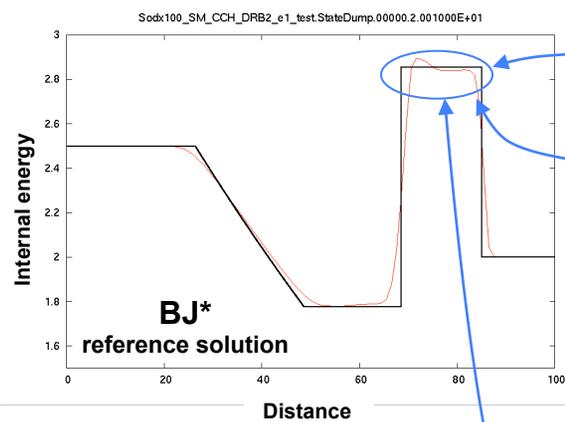
KE Velocity limited to make KE monotonic****

{ α, β }

Limiters for density & other variables are synchronized

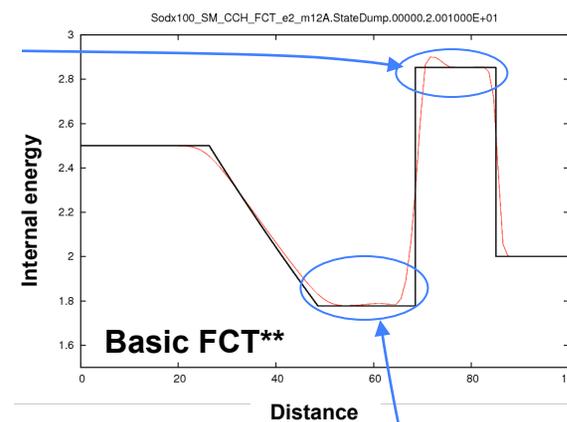
- * Barth, Jespersen 1989
- ** Zalesak 1979
- *** Schär, Smolarkiewicz 1996
- **** Liska, Shashkov, Vachal, Wendroff 2011

Comparison of monotonicity schemes on Sod problem – the BJ & basic FCT schemes may be “good enough”



FCT slightly better than BJ reference

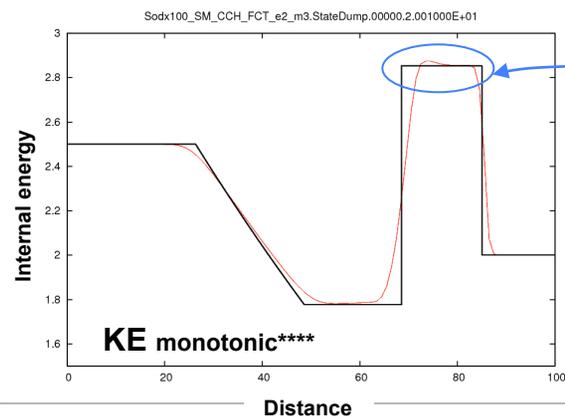
Overshoot due to wall heating at contact in Lagrange solution



Density limiter not synchronized

$$\beta \leq \frac{\mathbf{u}_a^{\max} M_a^L - \mathbf{U}_a^L}{\sum_i \delta^i \mathbf{U}}$$

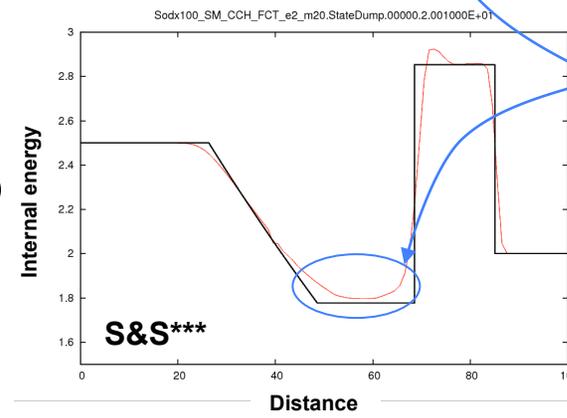
Typical form of the velocity limiter



KE reduces overshoot but is more dissipative

$$\beta \leq \frac{(\mathbf{u}_a^{\max} M_a^L)^2 - (\mathbf{U}_a^L)^2 - \sum_{i,j} \delta^i \mathbf{U} \cdot \delta^j \mathbf{U}}{2 \sum_i \mathbf{U}_a^L \cdot \delta^i \mathbf{U}}$$

Quadratic term needs further exploration



S&S more dissipative than FCT

$$\beta \leq \frac{\mathbf{u}_a^{\max} M_a^L - \mathbf{U}_a^L}{\sum_i \delta^i \mathbf{U} - \mathbf{u}_a^{\max} \sum_i \delta^i M}$$

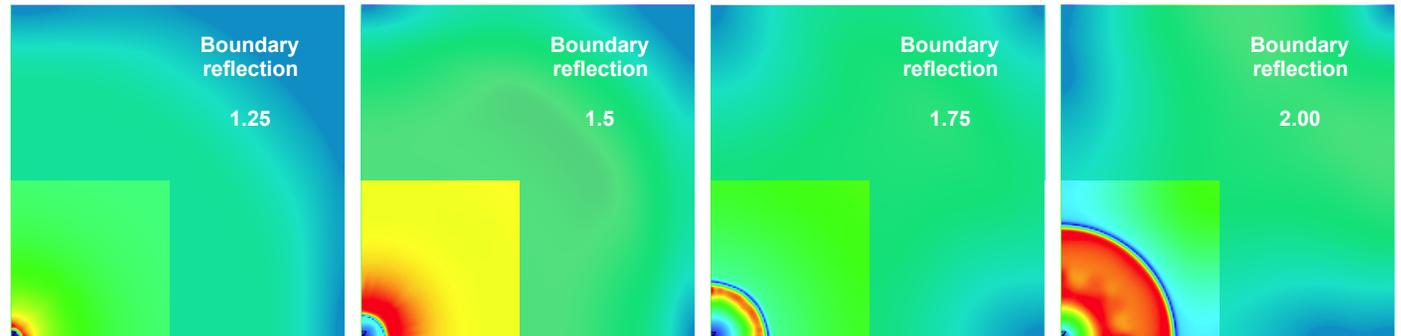
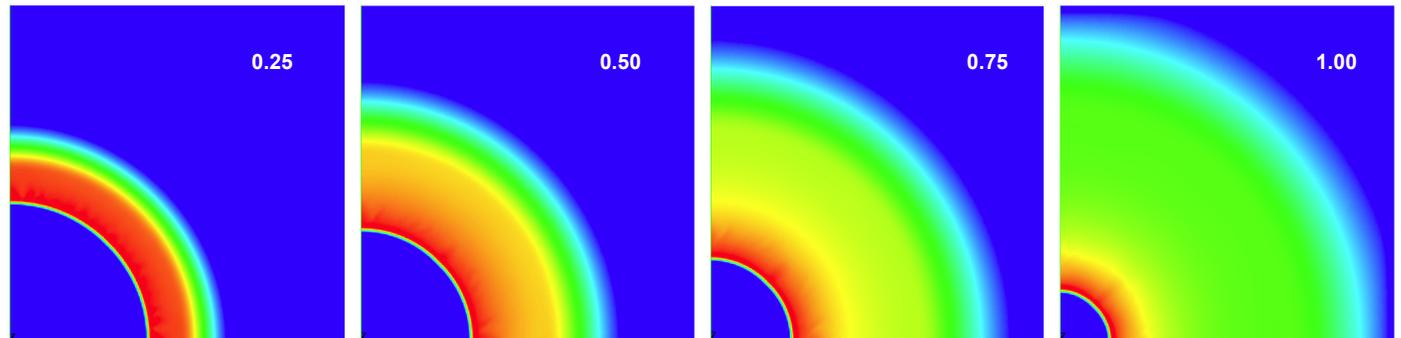
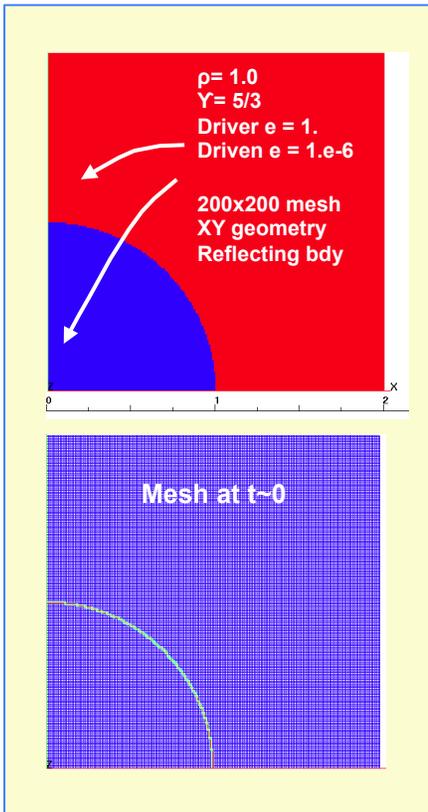
Density limiter synchronized with internal energy

- * Barth, Jespersen 1989
- ** Zalesak 1979
- *** Schär, Smolarkiewicz 1996
- **** Liska, Shashkov, Vachal, Wendroff 2011

The Convergent Sod problem is a variation of the “surrogate” Guderley problem* with a relatively small contact radius

The problem models a strong converging shock that reflects off the origin.

This is a CCH xALE (BJ+internal energy) calculation, showing velocity magnitude. Overall, the results are quite symmetric, but slight artifacts appear after shock reflection. How does this compare with other methods?



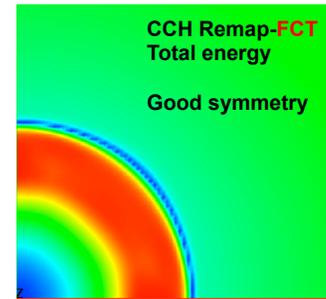
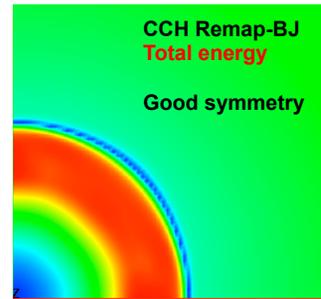
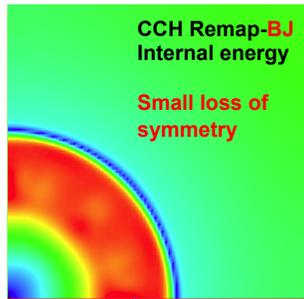
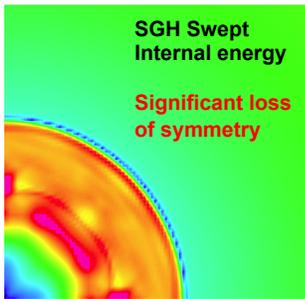
Shock reflects off the origin at about $t=1.3$

Slight asymmetry after shock reflects from the cavity surface at about $t=1.7$

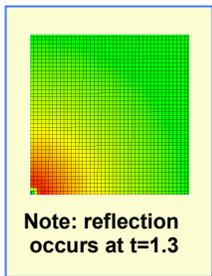
Boundary reflection interacts at about $t=2.0$

* Ramsey, Shashkov 2012
Kenamond, Bement, Shashkov 2012

A progression of algorithmic modifications highlights sensitivities in the Converging Sod problem

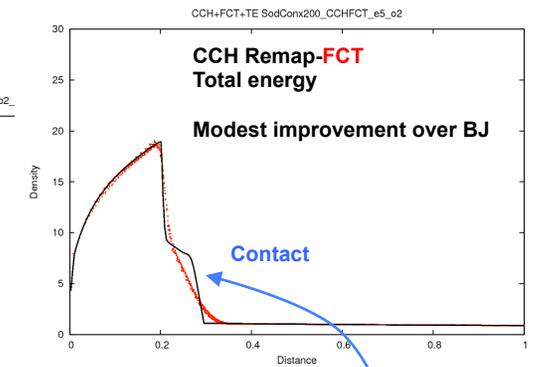
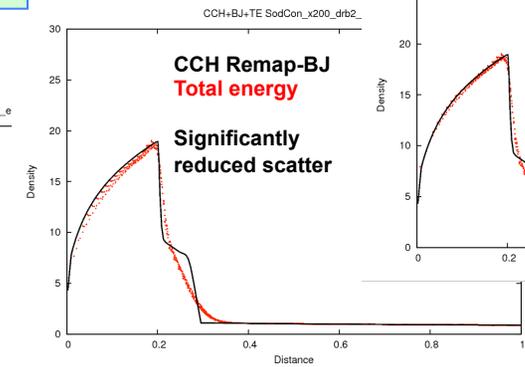
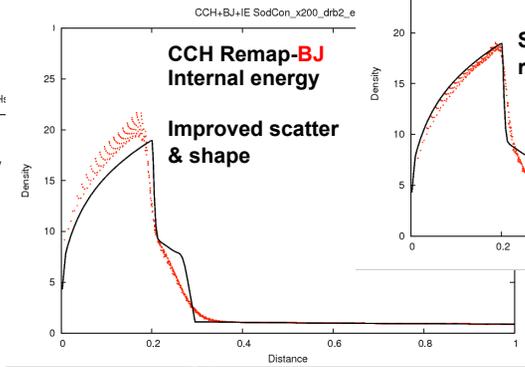
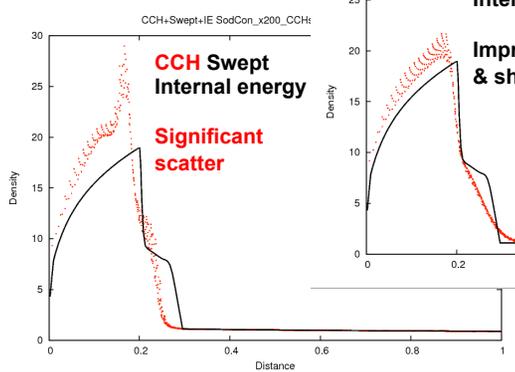
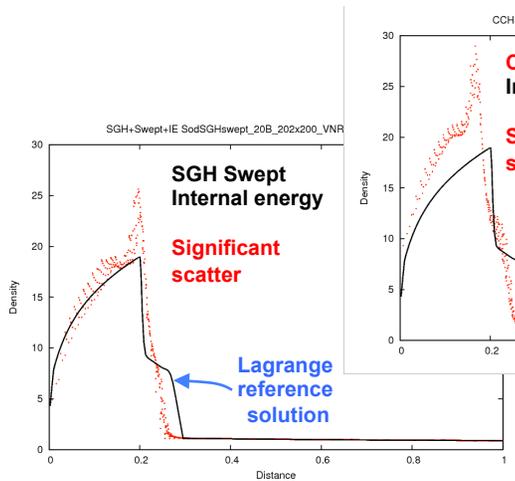


Velocity plots at t=1.8



Density vs radius scatter plots at t=1.6

Case from previous VG



Remap captures the outgoing shock very well

At this resolution, the Eulerian calculation does not capture the run up to the contact

Reference solution is a highly resolved 1D Lagrange SGH calculation

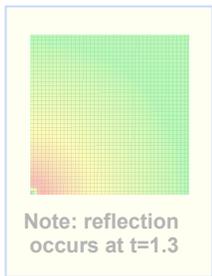
Conclusions:

- Total energy is essential
- FCT & BJ perform similarly

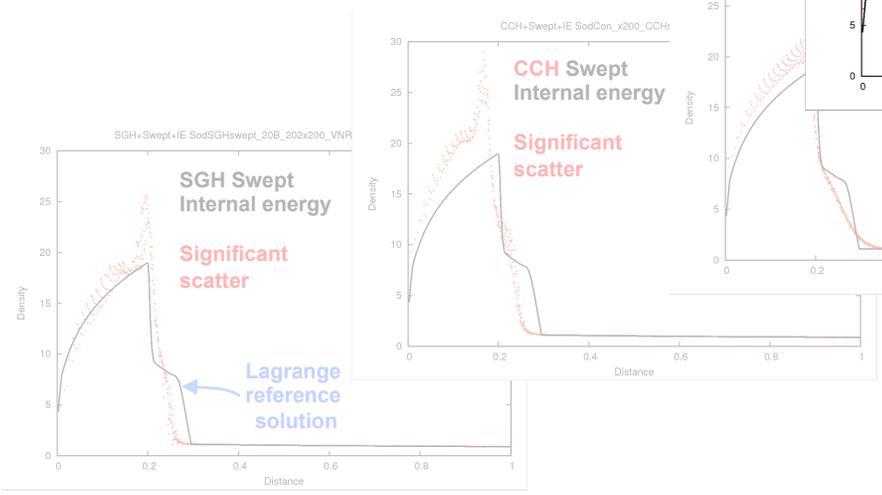
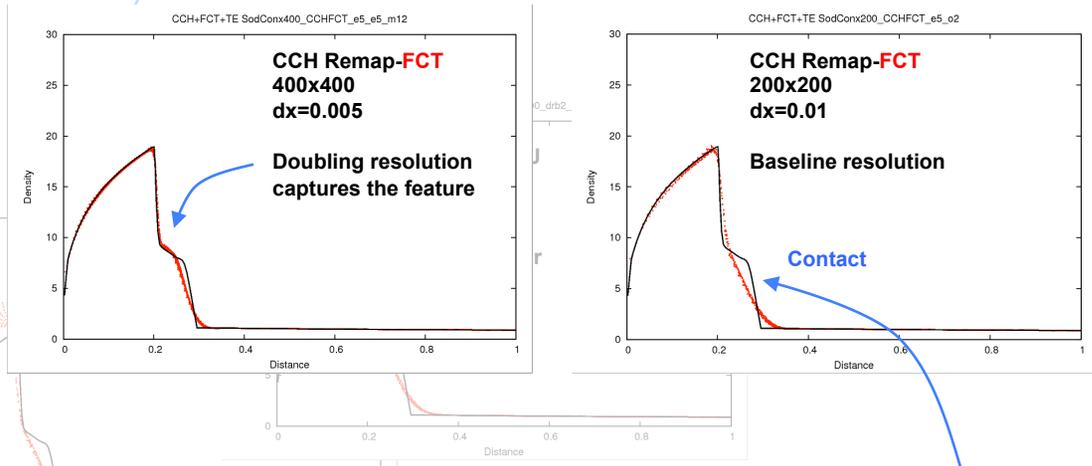
Increasing the resolution captures the feature



Velocity plots at t=1.8



Density vs radius scatter plots at t=1.6

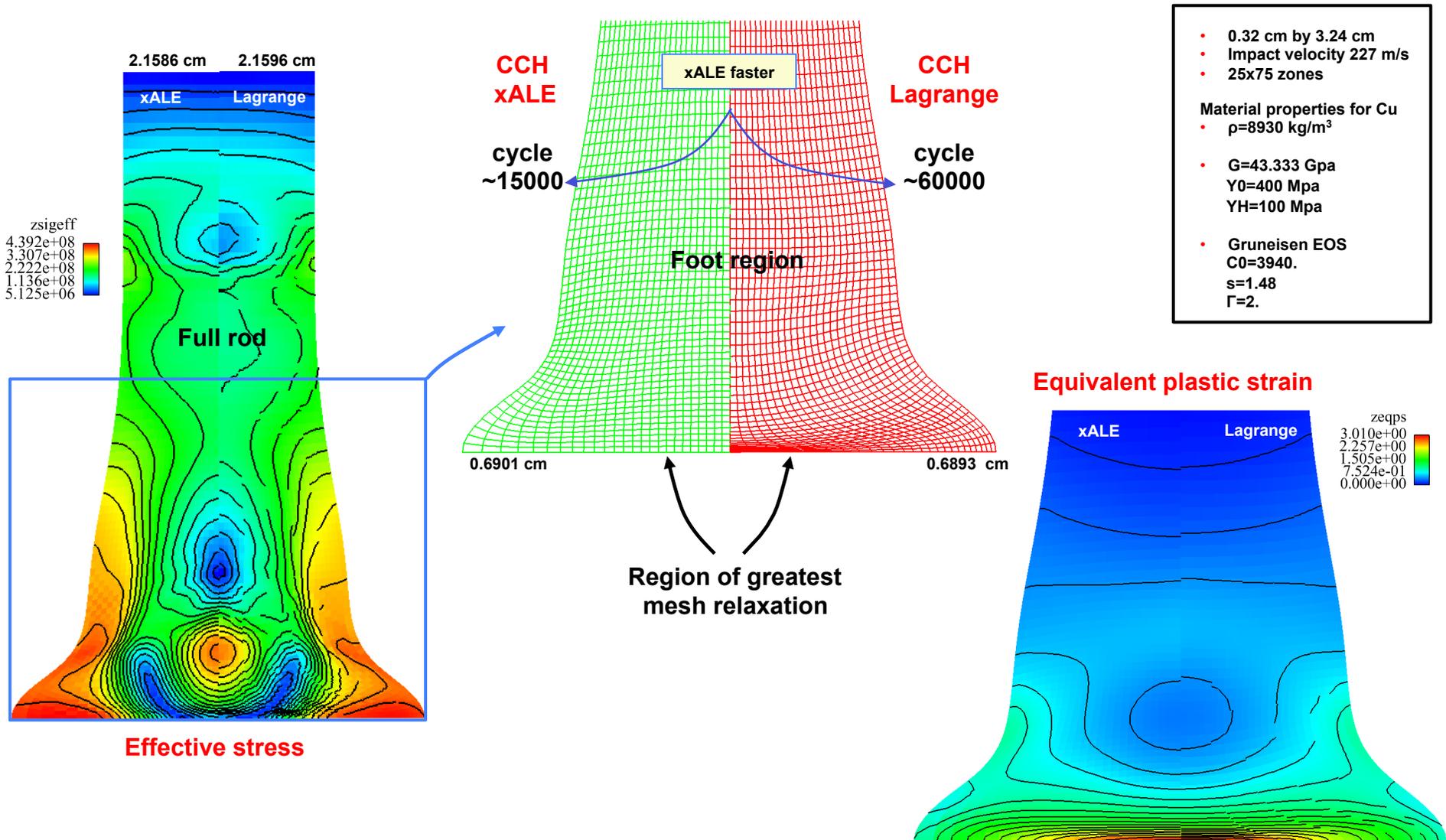


Remap captures the outgoing shock very well

At this resolution, the Eulerian calculation does not capture the run up to the contact

Reference solution is a highly resolved 1D Lagrange SGH calculation

Taylor anvil demonstrates xALE (BJ) with a solid strain-hardening model – xALE & Lagrange results are quite similar at 80 μ s



Burton, Carney, Morgan, Sambasivan, Shashkov, *Computers & Fluids*, 2012

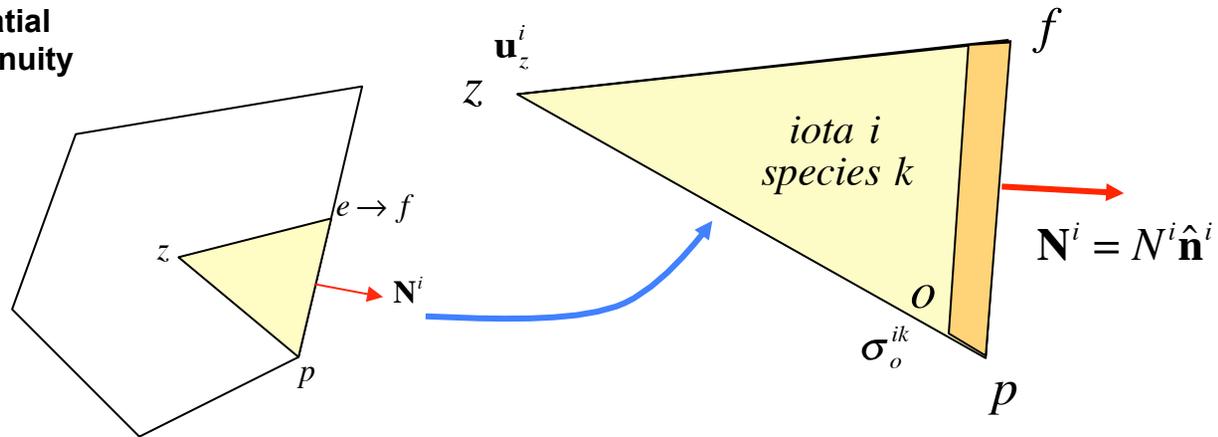
Multi-material

In the finite volume method, the integrals are replaced by sums of fluxes about the perimeter of the cell

The fluxes represent time and spatial averages. Consider volume/continuity equation

$$M_z \dot{y}_z = \oint_z d\mathbf{n} \cdot \mathbf{u}$$

$$\rightarrow \sum_i^z \mathbf{N}^i \cdot \mathbf{u}_p^i$$



in which the notation

$$\sum_i^z \mathbf{N}^i = 0$$

implies the sum of iotas about the zone or cell, and the sum about points is

$$\sum_i^p \mathbf{N}^i = 0$$

The basic connectivity structure is called an “iota”

Variables are located relative to the iota

\mathbf{u}_z^i is the cell centered velocity relative to iota i

σ_o^{ik} is the extrapolated stress tensor for species k and iota i

$\mathbf{N}^i = N^i \hat{\mathbf{n}}^i$ is the outward surface normal

The data structures generalize to 3D and collapse to 1D - so that the same code is executed in all dimensions

The fundamental multi-material assumption is that inter-species drag forces are sufficient to completely couple the momenta

Then, all species “ k ” have the same velocity but different thermodynamic states

Momentum

$$M_z \dot{\mathbf{u}}_z = \sum_{i,k} \varphi_z^{ik} \mathbf{N}_i \cdot \boldsymbol{\sigma}_p^{ik}$$

Mass & volume fractions

$$M_z = \sum_k M_z^k$$

$$\sum_k \varphi_z^k = 1$$

Closure model

Relaxes pressure

$$\delta_z^k V = \dots$$

$$\sum_{k,m} \delta_z^{km} V = 0$$

$$v_z^{k1} = \tilde{v}_z^{k1} + \frac{\delta_z^k V}{M_z^k}$$

& adjusts energy

$$\delta_z^k E = \dots$$

$$\sum_{k,m} \delta_z^{km} E = 0$$

$$e_z^{k1} = \tilde{e}_z^{k1} + \frac{\delta_z^k E}{M_z^k}$$

Volume

$$M_z^k \dot{v}_z^k = \sum_i \varphi_z^{ik} \mathbf{N}_i \cdot \mathbf{u}_p^i + \sum_m \delta_z^{km} V$$

$$= M_z^k \dot{\tilde{v}}_z^k + \delta_z^k V$$

Total energy

$$M_z^k \dot{t}_z^k = \sum_i \varphi_z^{ik} \mathbf{N}_i \cdot \boldsymbol{\sigma}_p^{ik} \cdot \mathbf{u}_p^i + \sum_m \delta_z^{km} E$$

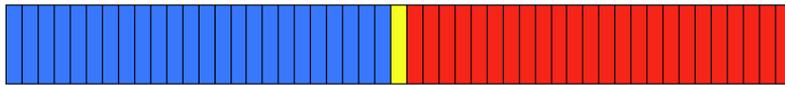
$$= M_z^k \dot{\tilde{t}}_z^k + \delta_z^k E$$

Here, we describe the Lagrange step

In remap, species are treated independently, but momenta are accumulated to form a conservative bulk velocity

D.E. Burton, T.C. Carney, N.R. Morgan, M.J. Shashkov 2011

In lieu of a composite EOS, we use a multi-species closure model – currently a variation of the Tipton* scheme adapted for CCH



$\rho_L = 1.0$
 $e_L = 2.0$
 $\gamma_L = 2.0$

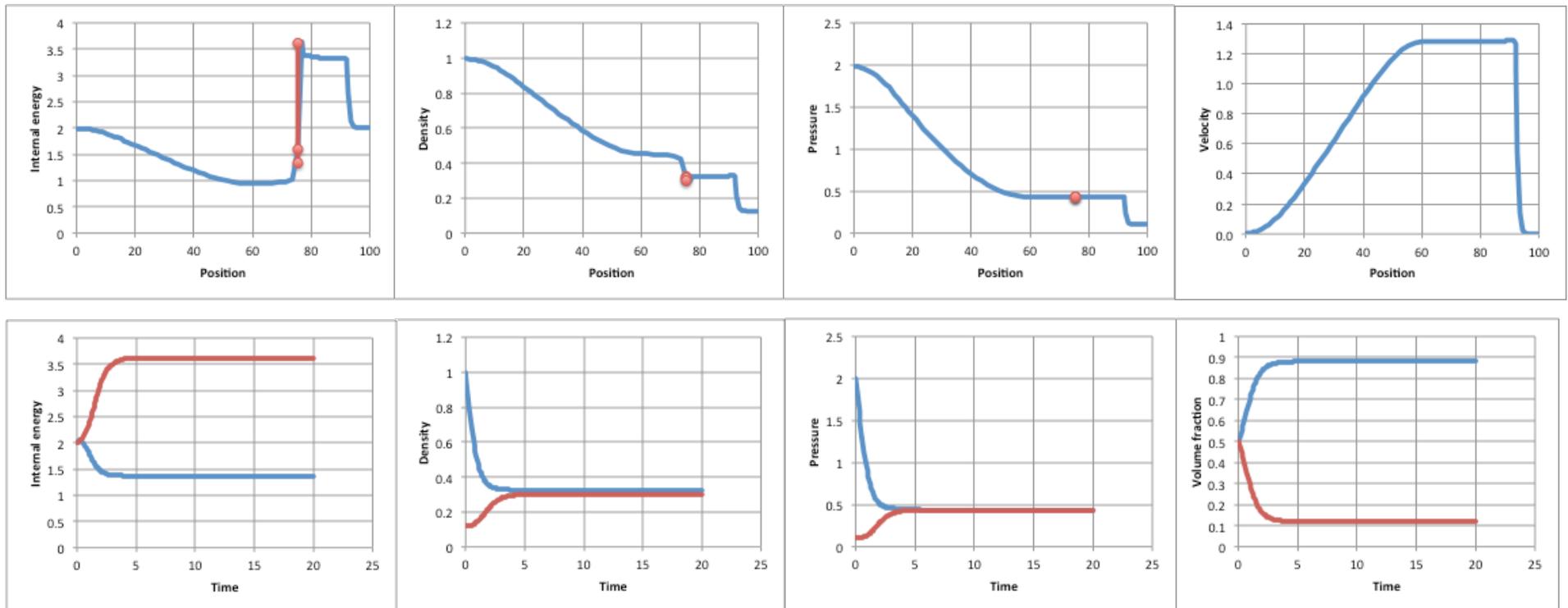
50:50 mixture

$\rho_R = 0.125$
 $e_R = 2.0$
 $\gamma_R = 1.4$

Performance on a 100 cell Sod problem**

** Specification:
LA-UR-12-22164
Francois, Shashkov,
Masser, Dendy

See Misha Shashkov's presentation for more elaborate closure models



- Transition to final state is essentially monotonic
- Transient averages (not shown) are bounded by L&R states

* Tipton 1989
Burton 2000 2012

In the multi-material nodal solution*, all species contribute to a single momentum equation, but each has its own stress

The stress field is discontinuous, so we must explicitly enforce conservation of momentum

Substitute the **dissipation relation** for each species k

$$\hat{\mathbf{n}}^i \cdot \boldsymbol{\sigma}_p^{ik} = \hat{\mathbf{n}}^i \cdot \boldsymbol{\sigma}_o^{ik} + \mu_c^{ik} (\mathbf{u}_p - \mathbf{u}_o^i) \left| \hat{\mathbf{n}}^i \cdot \hat{\mathbf{a}}_c^i \right|$$

into the **momentum conservation law**

$$0 = \mathbf{u}_p \sum_{i,k} N^i \varphi_z^{ik} \mu_c^{ik} \left| \hat{\mathbf{n}}^i \cdot \hat{\mathbf{a}}_c^i \right| + \sum_{i,k} N^i \varphi_z^{ik} \left[\hat{\mathbf{n}}^i \cdot \boldsymbol{\sigma}_o^{ik} - \mu_c^{ik} \mathbf{u}_o^i \left| \hat{\mathbf{n}}^i \cdot \hat{\mathbf{a}}_c^i \right| \right]$$

and solve for velocity directly

$$\mathbf{u}_p = \frac{\sum_{i,k} N^i \varphi_z^{ik} \left[\mu_c^{ik} \mathbf{u}_o^i \left| \hat{\mathbf{n}}^i \cdot \hat{\mathbf{a}}_c^i \right| - \hat{\mathbf{n}}^i \cdot \boldsymbol{\sigma}_o^{ik} \right]}{\sum_{i,k} N^i \varphi_z^{ik} \mu_c^{ik} \left| \hat{\mathbf{n}}^i \cdot \hat{\mathbf{a}}_c^i \right|}$$

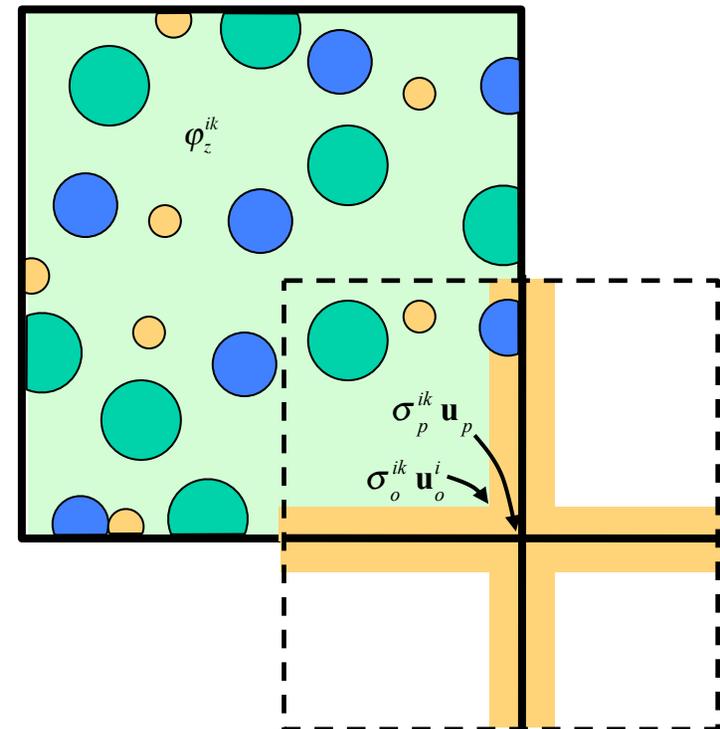
Calculate displacement

$$\mathbf{x}_p^1 = \mathbf{x}_p^0 + dt \mathbf{u}_p$$

and return to the dissipation relation to solve for the species stress components $\hat{\mathbf{n}}^i \cdot \boldsymbol{\sigma}_p^{ik}$

We do not assume a composite impedance in the nodal solution – nor do we assume a composite EOS

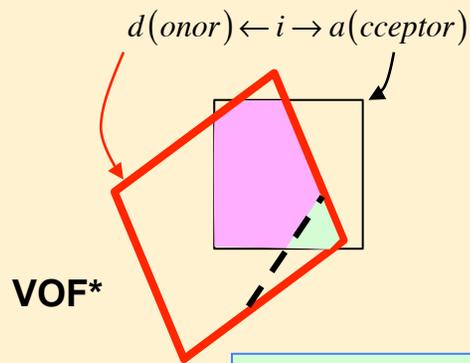
Doing so would lead to error in the species internal energy



* Despres, Mazeran 2005
Maire, Abgrall, Breil, Ovadia 2007
Burton, Carney, Morgan, Sambasivan, Shashkov 2011
Burton, Carney, Morgan, Sambasivan 2013

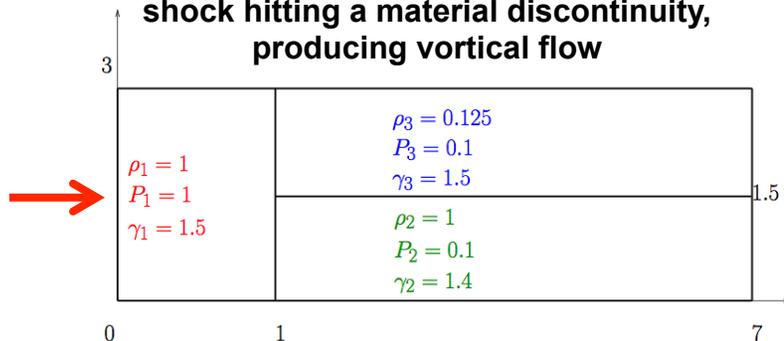
We are using an exact intersection VOF* treatment of material interfaces - Triple Point problem**

See Mack Kenamond's presentation for details of the VOF scheme



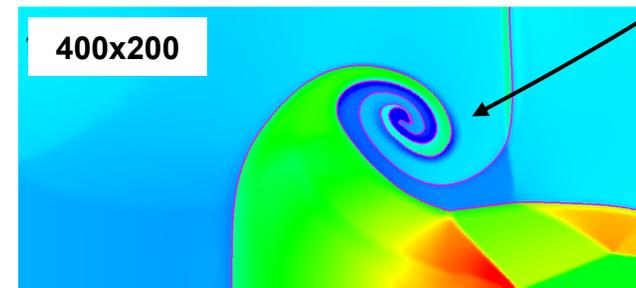
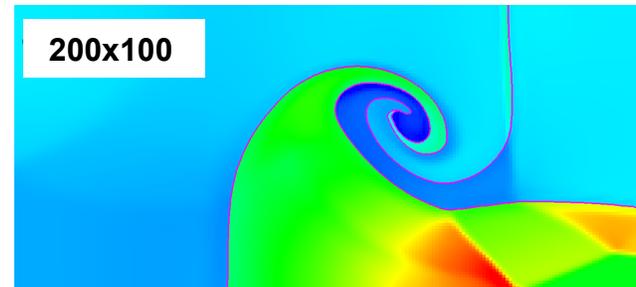
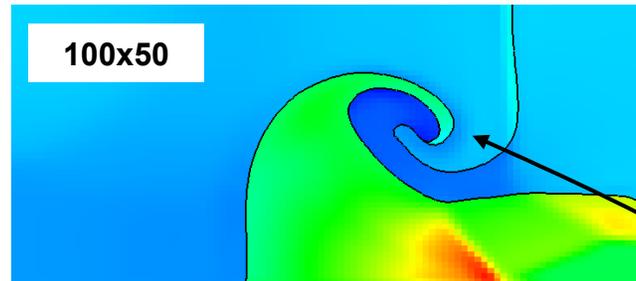
* Kenamond & Burton 2013
Mosso, Burton, Harrison 1998
Mosso, Burton 2000

The triple point problem simulates a shock hitting a material discontinuity, producing vortical flow



** R. Loubere et al 2010
Galera et al 2010

CCH+xALE (BJ) full Eulerian
(interface reconstruction & null closure)
t=5.0

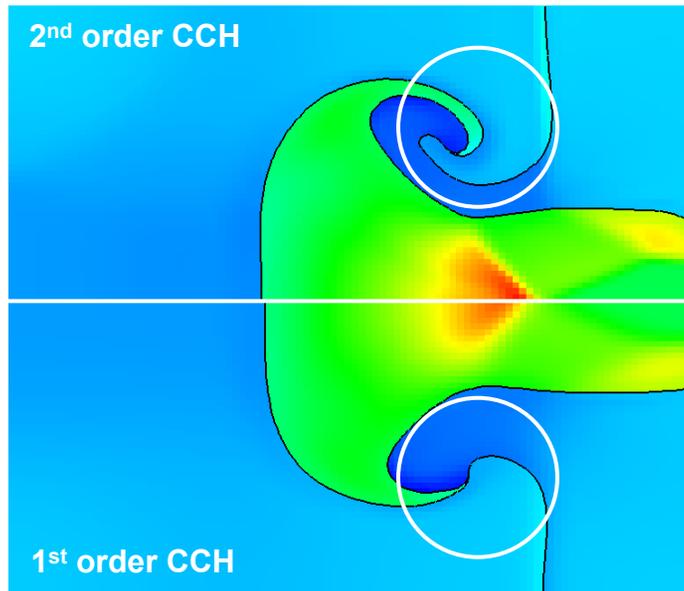


There is no converged solution.
Roll up should increase with resolution, until Kelvin-Helmholtz instabilities develop

Colors correspond to density on a quadratic scale from 0 to 3.

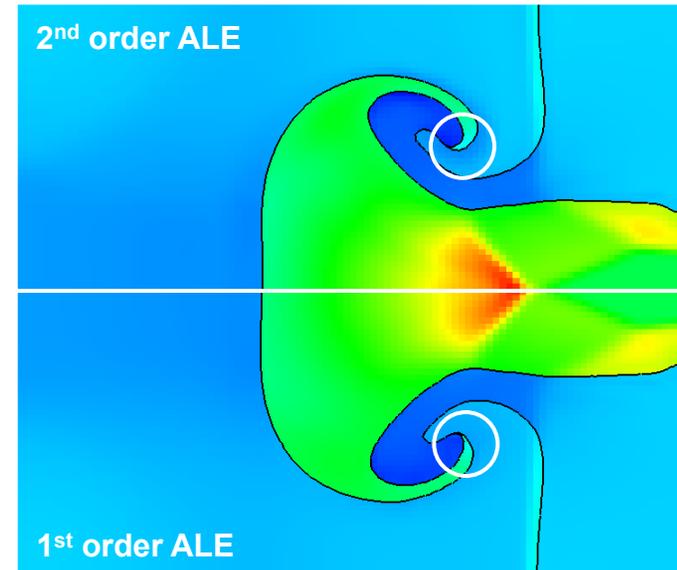
The order of the underlying hydro strongly affects the roll up

Order of underlying CCH hydro had a marked effect, roughly equivalent to doubling the resolution



2nd order ALE
Null closure
100x50

Order of the ALE scheme had only a minor effect on the solution for this problem



2nd order CCH
Null closure
100x50

Colors correspond to density on a quadratic scale from 0.1 to 5.0

Thoughts to take away

This presentation...

- Introduced an exact intersection remap scheme used with both single and multi-material cells and having computational cost $\sim n$
- Proposed an alternative to the canonical stress advection equation (elastic deformation/strain)
- Confirmed that, with bounds preservation of internal energy, the total energy based remap is superior to internal energy based remap
- Showed that major sources of error can be removed by using second-order remap and by enforcing total energy conservation
- Demonstrated Barth-Jespersen, basic FCT, and synchronized FCT methods for the remap of disparate grids (and not simply advection)
- Demonstrated application to solids
- Presented for multi-material cells:
 - multi-material evolution equations
 - multi-material nodal solution
 - multi-material remap
 - adaptation of the Tipton closure model to CCH
 - VOF

